

Preface

Quantitative structure–activity/property relationship (QSAR/QSPR) modelling has been used in medicinal chemistry and computational toxicology for a long time. It offers an *in silico* tool for the development of predictive models towards various activity and property endpoints of a series of chemicals using the response data that have been determined through experiments and molecular structure information derived computationally or sometimes from experiments. Once developed and validated, such models may be used for prediction of the response endpoint(s) for new and untested chemicals and also for obtaining a mechanistic interpretation of the structure–activity/property relationships. Although these techniques have been successful in many lead optimization and risk assessment problems, their use was previously limited to specific groups of researchers in the chemical sciences. With the easy availability of QSAR-related software tools, QSAR/QSPR modelling is now being exercised by a wider class of researchers; however, some of the users might not have proper background theoretical knowledge in the area. It is desired that QSAR/QSPR users should not depend solely on the available software for model development; *instead*, they should have a basic working knowledge of the theoretical aspects and principles of QSAR/QSPR modelling so that they can develop statistically valid and predictive models which can be meaningfully interpreted.

QSAR/QSPR of the present day is different from what it was during the initial days of its evolution in the form of “Classical QSAR”. With the introduction of newer (and higher dimensional) descriptors, the use of sophisticated chemometric tools and rigorous validation strategies and integration with other ligand and structure-based approaches, QSAR/QSPR of the present day is a recognized scientific discipline. QSAR/QSPR is also finding newer applications in diverse fields such as modelling properties/toxicities of nanomaterials, ionic liquids, chemical mixtures, cosmetics, etc., making this an area of potential interest.

In this brief, we aim at introducing the fundamental concepts of QSAR/QSPR modelling in a nutshell to students of Chemical Sciences. The basic concepts seeded into the mind of the students would be a *primer* for the development of their further knowledge in the area through practical modelling exercises and/or additional readings.

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Fundamental Concepts

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